

Reply to Comment on “Quantum phase transition in the four-spin exchange antiferromagnet”

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We argue that the analysis of the J-Q model, presented in Ref. 2 and based on a field-theory description of coupled dimers, captures properly the strong quantum fluctuations tendencies, and the objections outlined in Ref. 1 are misplaced.

In a recent paper, Isaev, Ortiz, and Dukelsky¹ have questioned the interpretation of our results on the J-Q model². In addition, they have argued that their hierarchical mean-field (HMF) method provides a more accurate description of the phase diagram of the model³. In our view the conclusions of Refs. 1,3 are highly questionable, and we address the two relevant issues below.

(1.) First, let us put our results (Ref. 2) in the correct perspective. In the notation of Ref. 1, let J_K be the 2-spin exchange and $-K$ be the 4-spin one; both J_K and K are assumed positive. These are the quantities we have used in our work, Ref. 2 (where we call J_K simply J). They are related to the couplings Q, J used in the original work of Sandvik⁴ via $Q/J = (K/J_K)/[1 - K/(2J_K)]$.

We prefer the J_K, K units, because this way we can make the ratio of the 4- to the 2-spin term arbitrarily large, whereas, for technical reasons, in the original work of Sandvik this ratio has a maximum value of $(K/J_K) = 2$, which corresponds to $Q/J = \infty$. If (K/J_K) is larger than 2, then this would mean $J < 0$, but still the 2-spin exchange in those units, $(J + Q/2)$, is positive. Now, Sandvik’s Monte Carlo (MC) result (confirmed also by later work^{5,6}), gives the critical value $(Q/J)_c \approx 25$, meaning $(K/J_K)_c \approx 1.85$. Our most advanced calculation finds the critical point at $(K/J_K)_c \approx 2.16$, which we argue to be an improvement relative to our simple mean-field value, which is $(K/J_K)_c^{MF} \lesssim 1$.

Our main point is that while our mean-field result gives $(K/J_K)_c^{MF} \lesssim 1$ (i.e. Q/J small, less than 2), our improvements, which take into account the strong quantum fluctuations, lead to $(K/J_K)_c$ around 2, meaning that $|Q/J| \gg 1$. We call these “weak”, and “strong” coupling regimes, respectively. In this sense our value $(K/J_K)_c = 2.16$ is in “fairly good agreement with the MC”, i.e. the critical point is firmly in the strong-coupling regime.

The authors of Ref. 1 object to the fact that our $(K/J_K)_c = 2.16$ corresponds to $(Q/J)_c = -27$, i.e. $J < 0$, which appears very far from the Monte Carlo: $(Q/J)_c = +25$, i.e. $(K/J_K)_c = 1.85$. However this a very misleading and incorrect way to look at the results

(that’s why we prefer the K, J_K units).

Since the transition is at large $|Q/J|$, it is irrelevant that $J < 0$. Indeed, the ratio of the 4- to the 2-spin term at our critical point, $(K/J_K)_c = 2.16$, corresponds to the 4-spin term being Q , and the 2-spin term being $(-|J| + Q/2)$, with $Q/|J| = 27$. Sandvik’s result, $(K/J_K)_c = 1.85$, means that the 4-spin term is Q , and the 2-spin term is $(J + Q/2)$, with $Q/J = 25$.

In both cases $|Q/J| \gg 1$, so the sign of J is irrelevant. This is what we call the strong-coupling regime, when K/J_K is around 2, and we describe the agreement between $(K/J_K)_c = 1.85$ and $(K/J_K)_c = 2.16$ as “fairly good”. The two critical points are fairly close, when things are put in the right context. We have certainly not achieved a perfect agreement with the Monte Carlo, but we have found the correct quantum fluctuations trend.

Of course, as pointed out in Ref. 1, the point $(K/J_K)_c = 2.16$ is outside the range explored in the work of Sandvik⁴, but the physics is expected to be the same, i.e. one simply penetrates deeper into the quantum disordered, gapped phase.

(2.) We also emphasize that our results were obtained under the assumption that the ground state is of the columnar dimer type, as argued in Ref. 4. In our work we found that this ground state is stable for $K/J_K > (K/J_K)_c$, but we did not compare with other possible ground states, as it is quite difficult to compare ground state energies reliably⁷, especially when the system exhibits strong fluctuations.

A severe problem of the HMF approach³ is that the critical point is at $(Q/J)_c \approx 2$, i.e. $(K/J_K)_c \approx 1$, which is far off the Monte Carlo result. In fact the HMF critical point location is close to the one we found in our “simple” dimer mean-field framework², which we ruled out as unreliable. Thus the hierarchical plaquette mean-field seems to place the critical point firmly in the weak-coupling (small Q/J) region, in disagreement with the Monte Carlo, and consequently it is highly unlikely that the HMF takes properly into account the strong quantum fluctuations present in the J-Q model.

¹ L. Isaev, G. Ortiz, and J. Dukelsky, arXiv:1003.5205.

² V. N. Kotov *et al.*, Phys. Rev. B **80**, 174403 (2009).

- ³ L. Isaev, G. Ortiz, and J. Dukelsky, J. Phys.: Cond. Matter **22**, 016006 (2010).
- ⁴ A. W. Sandvik, Phys. Rev. Lett. **98**, 227202 (2007).
- ⁵ R. G. Melko and R. K. Kaul, Phys. Rev. Lett. **100**, 017203 (2008).
- ⁶ A. W. Sandvik, Phys. Rev. Lett. **104**, 177201 (2010).
- ⁷ V. N. Kotov *et al.*, Phys. Rev. Lett. **80**, 5790 (1998).